NCEMSS - a program for simulation of HRTEM images

1. Introduction to the simulation process

1.1 Why simulate images ?

Image simulation grew out of an attempt to explain why electron microscope images of complex oxides sometimes showed black dots in patterns corresponding to the patterns of heavy metal sites in complex oxides, and yet other images sometimes showed white dots in the same patterns. This first application was therefore to characterize the experimental images, that is to relate the image character (the patterns of light and dark dots) to known features in the structure.

Most simulations today are carried out for similar reasons, or even as a means of structure determination. Given a number of possible models for the structure under investigation, images are simulated from these models and compared with experimental images obtained on a high-resolution electron microscope. In this way, some of the postulated models can be ruled out until only one remains. If all possible models have been examined, then the remaining model is the correct one for the structure. For this process to produce a correct result, the investigator must ensure that all possible models have been examined, and compared with experimental images over a wide range of crystal thickness and microscope defocus. It is also a good idea to match simulations and experimental images for more than one orientation.

Some simulations are done in order to throughly explore one particular image by "freeze-framing" the imaging process in the computer. In this way, we can obtain information that is not observable experimentally, such as the electron wave amplitude at the exit surface of the specimen, the magnitude and phase of each component of the image intensity spectrum, or even the amplitude contributed to the intensity spectrum by each pair of diffracted-beam interferences.

The simulation programs can also be used to study the imaging process itself. By simulating images for imaginary electron microscopes, we can look for ways in which to improve the performance of present-day instruments, or even find that the performance of an existing electron microscope can be improved significantly by minor changes in some instrumental parameter. Alternatively, based on imaging requirements revealed by test simulations, we can adjust the electron microscope to produce suitable images of some particular specimen, or even of some particular feature in a particular specimen.

1.2 Describing the transmission electron microscope

In order to simulate an electron microscope image, we need firstly to be able to describe the electron microscope in such a way that we can model the manner in which it produces the image. As a first step, we can consider the usual geometrical optics depiction of the transmission electron microscope (TEM).

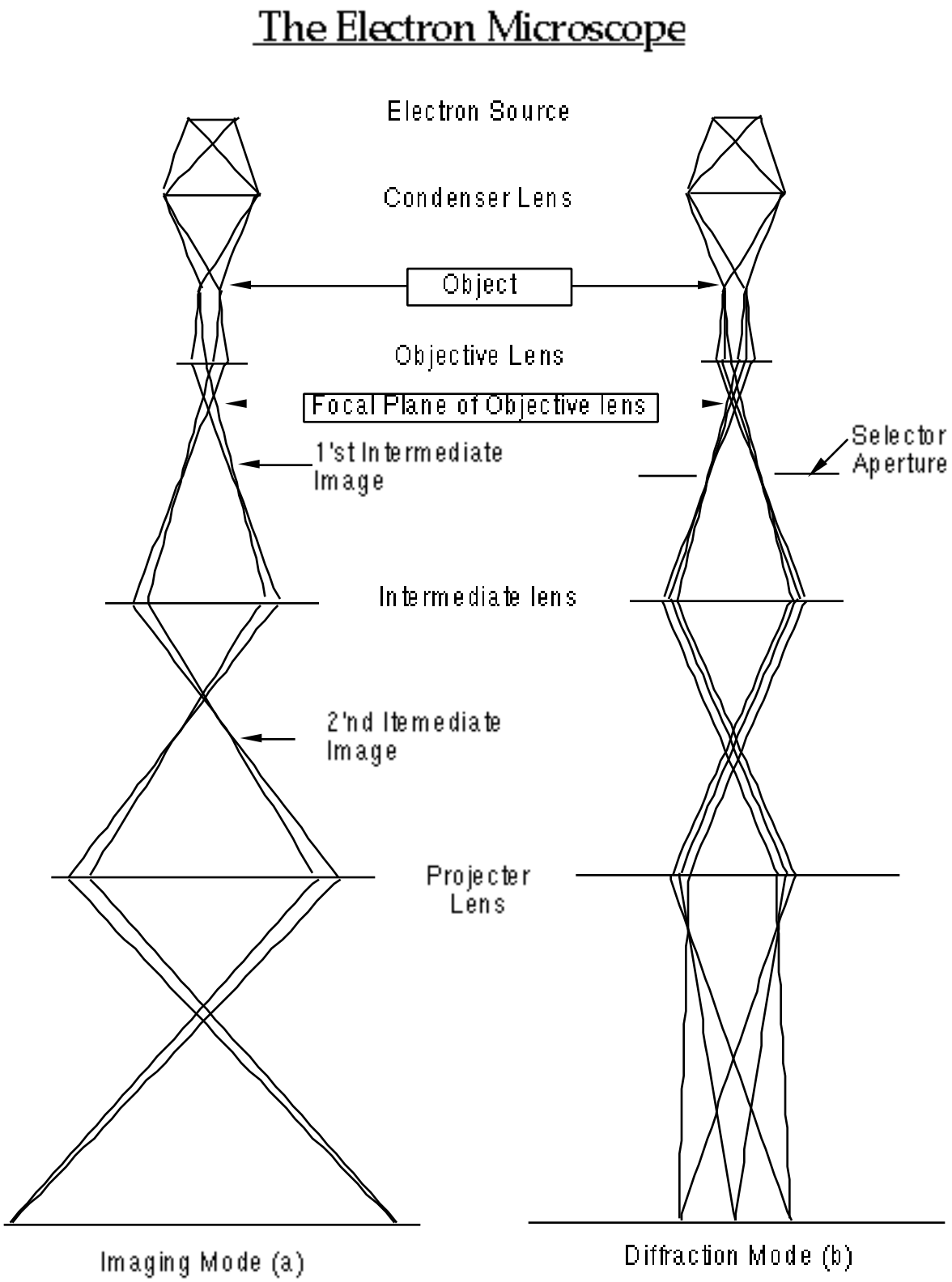

Fig.1 Geometrical optics representation of the TEM in imaging mode (a), and diffraction mode (b).

Figure 1 shows such a diagram of a TEM operated in two distinct modes, set up for microscopy (a), and for diffraction (b). In microscopy mode we see that the TEM consists of an electron source producing a beam of electrons that are focused by a condenser lens onto the specimen; electrons passing through the specimen are focused by the objective lens to form an image called the first intermediate image (I1); this first intermediate image forms the "object" for the next lens, the intermediate lens, which produces a magnified image of it called the second intermediate image (I2); in turn, this second intermediate image becomes the "object" for the projector lens; the projector lens forms the greatly-magnified final image on the viewing screen of the microscope. In microscopy mode, electrons that emerge from the same point on the specimen exit surface are brought together at the same point in the final image.

At the focal plane of the objective lens, we see that electrons are brought together that have left the specimen at different points but at the same angle. The diffraction pattern that is formed at the focal plane of the objective lens can be viewed on the viewing screen of the TEM by weakening the intermediate lens to place the microscope in diffraction mode (b).

1.3 Simplifying the description of the TEM

Consideration of the description of the electron microscope in figure 1 shows that the projector lens and the intermediate lens (or lenses) merely magnify the original image (I1) formed by the objective lens. For the purposes of image simulation we can reduce the TEM to three essential components; (1) an electron beam that passes through (2) a specimen, and then through (3) an objective lens (fig.2).

Our next step in describing the electron microscope for image simulation is to move from the geometrical optics description of the TEM to a description based on wave optics. In this description of the microscope we examine the amplitude of the electron wavefield on various planes within the TEM, and attempt to determine how the wavefield at the viewing screen comes to contain an image of our specimen.

By treating the electrons as waves, and considering our simplified electron microscope (fig.2), we see that there are three planes in the TEM at which we need to be able to compute the (complex) amplitude of the electron wavefield.

(1) The image plane:
Working backwards, we start with our desired information, the electron wavefield at the image plane; this wavefield is derived from the wavefield at the focal plane of the objective lens by applying the effects of the objective aperture and the phase changes introduced by the objective lens.

(2) The focal plane of the objective lens:
In turn, the electron wavefield at the focal plane of the lens is derived from the wavefield at the exit surface of the specimen by a simple Fourier transformation.

The Reduced Electron Microscope

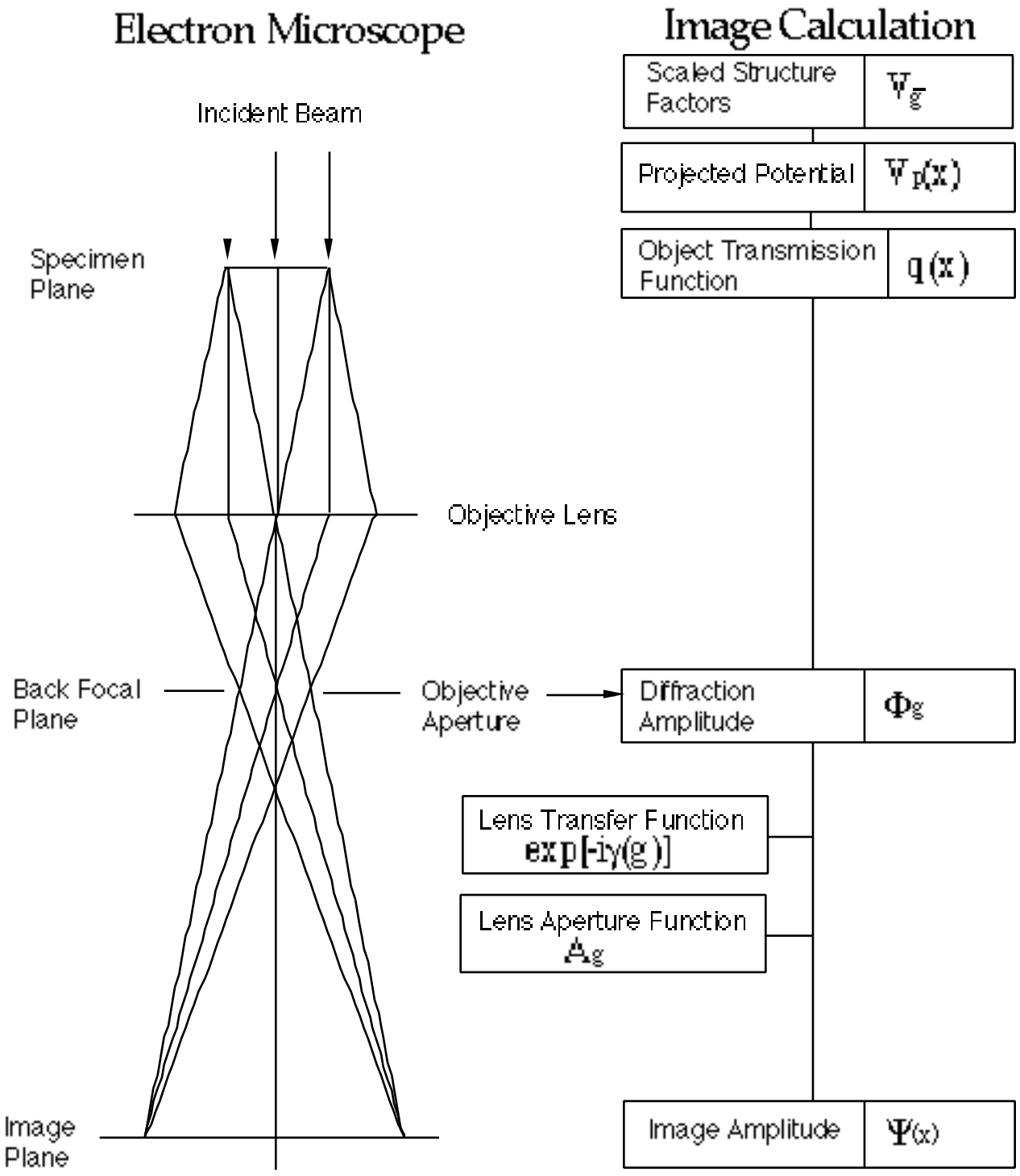

Fig. 2. The simplified TEM (left) and the calculations required for an image simulation (right). The three principal planes are marked.

(3) The specimen exit surface:
In order to know the exit-surface wavefield, we must know with which physical property of the specimen the wave interacts, and describe that physical property for our particular specimen.

Cowley and Moodie (1957) showed that the interaction of an electron beam with a specimen could be described by the so-called multislice approximation, in which electrons propagate through the specimen and scatter from the crystal potential; the electron scattering is described by the so-called phase-grating function, a complex function of the potential, and the electron propagation is computed with a propagation function dependent on the electron wavelength.

1.4 Simulating TEM images

The problem of simulating images thus becomes a problem of computing the electron wavefields at the three microscope planes. Currently, the best way to produce simulated images is to divide the overall calculation into three parts:

(1) Model the specimen structure to find its potential in the direction of the incident beam.

(2) Produce the exit-surface wavefield by considering the interaction of the incident electron wave on the specimen potential.

(3) Compute the image-plane wavefield by imposing the effects of the objective lens on the specimen exit surface wave.

Cowley J.M. & Moodie A.F. (1957) The scattering of electrons by atoms and crystals. I. A new theoretical approach. Acta Cryst. 10, 609.

2. Introduction to NCEMSS

2.1 The three simulation steps

Since the simulation problem divides neatly into three parts, NCEMSS treats these three parts with three sub-programs -

(1) PHSGRT - a program to generate the part of the crystal potential that produces electron scattering; input is from a file containing structural data about the specimen, including unit cell dimensions, symmetries, and atom positions, occupancies, and temperature factors.

(2) MSLICE - a program to generate the electron wavefield at the specimen exit surface; it uses PHSGRT data combined with information about the accelerating voltage of the electron microscope, and the specimen thickness and tilt.

(3) IMAGE - a program to generate the image intensity at the microscope image plane; the effects of objective lens phase changes and resolution-limiting aberrations are included via parameters like defocus, spherical aberration, incident beam convergence, spread-of-focus, and the position and size of the objective aperture.

Thus PHSGRT considers only the specimen structure, MSLICE treats the interaction of the specimen with the electron wave, and IMAGE simulates how the wave leaving the specimen interacts with the lens system of the electron microscope. Once a simulation has been made, any additional simulation will usually not require a full re-simulation; any change in microscope parameters will not affect the results of the PHSGRT and MSLICE programs, and only IMAGE will need to be re-run; any change in microscope voltage or in specimen thickness or tilt will not affect the results of PHSGRT, but MSLICE and IMAGE will need to be re-run. Of course, any change in the specimen structure will require the re-running of all three subprograms.

2.2 NCEMSS files

Supplied files: NCEMSS uses four data files to store supplied information not normally altered by the user:

(1) **spcgrp.dat** stores information on all 230 space groups for generation of crystal symmetry operators as required by the input specimen structures.

(2) **scatt.dat** stores information on atomic scattering factors for the first 98 elements.

(3) **microscopes.dat** stores information on the imaging parameters of various high-resolution electron microscopes. Note that the user has the option of adding additional microscopes to the table stored in MICROSCOPES.DAT.

(4) **lprint.ps** stores a set of Postscript definitions that are used in order to print images to a Postscript Laserprinter.

Generated files: NCEMSS generates and stores various data files in the course of a simulation. The five data files are:

(1) **name.at** stores all the structure and microscope information needed to run the simulation. This information is derived from user input and the supplied data files. In particular, the string "**name**" is a unique name for the structure, input by the user when creating the structure file.

(2) **name.pout** is the result of running the PHSGRT subprogam from the information stored in *name.at*; it contains the specimen potential in the direction of the electron beam.

(3) **name.mout** is the result of running the MSLICE subprogram using the data in *name.pout* with those in *name.at*; it contains the exit-surface wave at one or more selected specimen thicknesses.

(4) **name.iout** is the result of running the IMAGE subprogram to apply the effects of the microscope parameters in the *name.at* file to the exit-surface wave; it contains one or more images ready to be displayed.

(5) **name.aout** contains the complex amplitudes of several diffracted beams at one-slice increments in specimen thickness. The beams are specified by the user in the main menu, and can be plotted as a function of specimenthickness.

In addition, two print files are produced (but rarely printed) just in case additional information about a computation is required by the user. These files are:

(6) **name.p_prnt** contains information about the way in which the PHSGRT subprogram processed the *name.at* data to produce the specimen potential.

(7) **name.m_prnt** contains information about the way in which the MSLICE subprogram processed the *name.pout* data with *name.at* data to produce the exit-surface wave; that is, it contains information on the multislice computation.

Since NCEMSS images are stored in a file for interactive display, the user has the option of writing any image to the display screen with any selected number of unit cells, with any selected value of contrast and brightness, and at any selected magnification. In addition, the user may elect to display (i.e. write to the screen) real-space functions like the projected crystal potential, the exit-surface electron wavefunction, or a drawing of the atom positions; in addition, reciprocal-space functions such as the diffraction intensities and the image power spectrum ("optical" diffractogram) may be displayed and indexed.